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Young's Modulus of Nano Polycrystalline Silicon Film

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Abstract

To apply the nano polycrystalline silicon film (NPSF) to MEMS piezoresistive device effectively, the Young's modulus of the NPSF were tested by in-situ nano mechanical test system, the results show that the Young's modulus of the NPSF is about between 155GPa and 158GPa. According to the specialties of growing and structure of the nano polycrystalline film materials, a theoretical model was presented which is suitable for NPSF. The Young's modulus of the NPSF was calculated by the model, the theoretical result agrees with the experimental result. The theory model is valid and can be applied to analyses of the Young's modulus of other nano polycrystalline film materials.

Nano polycrystalline silicon film, Young's modulus, MEMS

1. Introduction

The researches about nano materials developed rapidly in 21st century [1]. Nano material is a kind of material in which one of the material's dimensions is in nanoscale (1~100nm). Nano material can be sort into 3 kinds, including zero dimension, one dimension and two dimension. Two dimension nano materials is a kind of film whose thickness is less than 100nm, i.e. nano film [2]. In this paper, polycrystalline silicon film whose thickness is under 100nm is called nano polycrystalline silicon film (NPSF),

To utilize the NPSF further, the Young's modulus of NPSF with 60nm and 90nm thickness were tested by in-situ nano mechanics test system TriboIndenter. According to the structure characteristics of NPSF, a theory model is presented. The Young's modulus of NPSF is calculated by the model, the comparison between theoretical result and experimental result is conducted.

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2. Experimental

The 4 inch monocrystalline silicon wafers (thickness: 500μm) of <100> orientation were chosen as substrates, then a $Si0_2$ layer (thickness: 1μm) grown by thermal oxidation. The oxidation layer can insulate the substrate and NPSF. The NPSF were deposited at 620℃ with SiH_4 flow rates 50ml/min in a low pressure chemical vapor deposition system. The thicknesses of NPSF are controlled by deposition time. The film thickness is 60 nm and 90nm, respectively, and error of the thickness is about ±3nm. Then using boron nitride of solid state, the thermal diffusion was processed at 1080℃ with nitrogen protection; the doping concentration of both NPSF is estimated to be $2.3x10^{20}cm^{-3}$ in terms of solubility of solid-state boron in silicon. In this step, the NPSF finished annealing also. Test samples (10mm×10mm) were obtained through photolithography. The samples are for testing of Young's modulus of NPSF. On the other hand, 10mm×10mm square $Si0_2$ film (thickness: 100nm) samples were prepared for comparison in measurement of Young's modulus also.

3. Results

In-suit nano mechanics test system TriboIndenter can be use to measure the mechanics parameters of material, including Young's modulus, hardness, frictional coefficient, dynamic stiffness and loss modulus. We utilized the system to test Young's modulus of square samples of NPSF and $Si0_2$ film. By loading control of auto mode, TriboIndenter fulfill the continuous loading and unloading of materials. The Young's modulus of material can be calculated by analyses of loading-unloading curve obtained from the experiments. In this paper, the methods and theoretical formulas [4] in the calculation are neglected; we only present the loading-unloading curves and corresponding experimental results.

The square samples of 60nm NPSF were tested many times, and the typical loading-unloading curve is shown in Fig.1. From the figure, the Young's modulus of 60nm NPSF is calculated to be 155GPa.

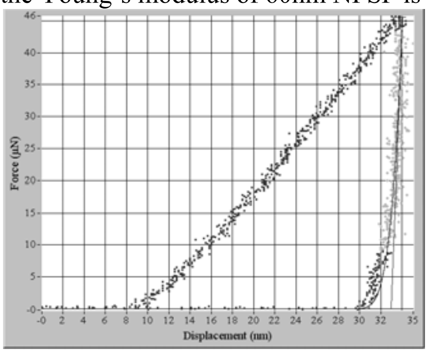

Fig. 1. Loading-unloading curve of square sample of 60nm NPSF

In the same way, the square samples of 90nm NPSF were tested also, and the typical loading-unloading curve is shown in Fig.2. From the figure, the Young's modulus of 90nm NPSF is calculated to be 158GPa.

For comparison, the square sample of 100nm $Si0_2$ film were tested in the test process of 60nm and 90nm NPSF. The typical loading-unloading curve is shown in Fig.3. From the figure, the Young's modulus of 100nm $Si0_2$ film is calculated to be 73.56GPa.

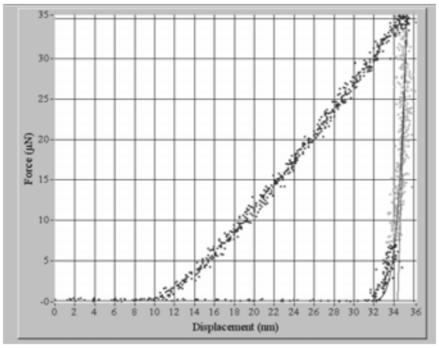

Fig. 2. Loading-unloading curve of square sample of 90nm NPSF

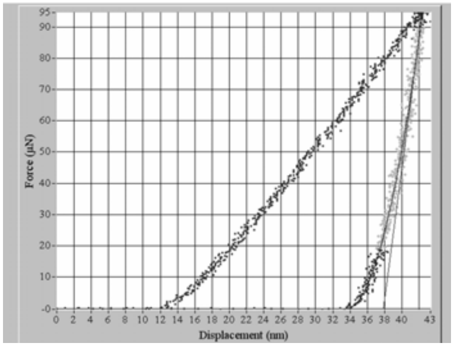

Fig. 3. Loading-unloading curve of square sample of 100nm SiO_2 film

4. Discussion and Analyses

From Fig. 1 and Fig. 2, the Young's modulus of NPSF is between 155GPa and 158GPa, and decrease lightly with thickness of NPSF decreasing. The Young's modulus of NPSF is smaller than that of common polycrystalline silicon film (CPSF), which is 163GPa, representatively [7]. Along with decreasing of film thickness, the trap density in grain boundary and defect increase, the rigidity of grain boundary decrease; and at the same time, the grain size decrease, the weight of grain boundary on grain unit increase, the rigidity of film decrease, so the Young's modulus of the film decrease.

As we known, the Young's modulus of $Si0_2$ is about 73GPa [8]. In our experiments, the Young's modulus of 100nm $Si0_2$ film is calculated to be 73.56GPa, which is very close to the known value. It indirectly proves that the testing method of the Young's modulus of NPSF is valid, the experimental results is credible.

In following, a theory model is presented to investigate the Young's modulus of NPSF, which is fit to nano polycrystalline film materials also. In structure, the NPSF is composed of monocrystalline silicon grains with different crystalline orientations, every grain can be seen to be a single crystalline silicon unit. Around the units, amorphous silicon fills the interspaces between the units, and there are lots of defects and .dangling bonds, i.e. grain boundary. In general, the width of grain boundary is less than 1nm.

Because of the insulator layer between the NPSF and substrate, the growth of NPSF is independent of substrate, and preferred orientation of NPSF is independent of orientation of the substrate also. The previous researches show that [100] preferred orientation usually exist in only CPSF with bigger thickness [9]. According to our previous researches, for NPSF prepared in our experiments, no obvious preferred orientation exists.

Macro elastic constant of polycrystalline materials is close related to elastic constant of grains and ways of grains making up of polycrystalline materials. Because no preferred orientation exists in the NPSF, and it is isotropic in film plane unless the NPSF is annealed by laser and electron beams [10], a theory model of NPSF is presented, and the key points of the model are followed: 1. Because of very thin thickness of NPSF, grains arrange in single layer in the film plane, the vertical height of grains is equal to the thickness of NPSF. 2. The grain size of NPSF is very bigger than width of grain boundary, so the effect of grain boundary on elastic constant of grain unit is neglected, where grain boundary rigidly connect grain units. 3. In the film plane of NPSF, orientation distribution of grain is symmetrical; every grain can find another grain where orientation is symmetrical with each other, the isotropy in film plane can be guaranteed. 4. For NPSF, the grains grow randomly; the orientation distribution of grain is random also. No preferred orientation exists in NPSF.

According to the key points 1 and 2 of the model, if there is strain exist in film, every grain should receive the same strain, i.e. uniform strain distribution. Assumed any grain of NPSF receives strain is $\varepsilon^i = \varepsilon, i = 1 \cdots N$, where the parameter N is total number of grains in NPSF. So average strain of the NPSF is $\overline{\varepsilon} = \varepsilon$. Because of different orientation of every grain, the Young's modulus of every grain is different also, so every grain receives different stress. Assumed the Young's modulus of any grain is Y^i, the stress received by any grain is $\sigma^i = Y^i \varepsilon$.

So average stress of NPSF is followed:

$$\overline{\sigma} = \frac{1}{N}\sum_{i=1}^{N}\sigma^i = \varepsilon\frac{1}{N}\sum_{i=1}^{N}Y^i \quad \text{s} \tag{1}$$

If the Young's modulus of the film is defined to be the ratio of average stress and average strain, we have:

$$\overline{Y} = \frac{\overline{\sigma}}{\overline{\varepsilon}} = \frac{1}{N}\sum_{i=1}^{N}Y^i \tag{2}$$

From equation (2), the Young's modulus of NPSF is mean of Young's modulus of all grains in film.

For NPSF, the planar size of film is usually from several decades to several hundred microns, in contrast the grain size is only several decades nanometer. The total number of grain is very large, i.e. parameter N in equation (2) is very large, and so the summation can translate into integrating, as followed:

$$\overline{Y} = \frac{1}{N}\sum_{i=1}^{N}Y^i = \frac{\int_0^{2\pi} Y(\theta,\varphi)D(\theta,\varphi)d\Omega}{\int_0^{2\pi} D(\theta,\varphi)d\Omega} \tag{3}$$

Where Ω is solid angle, $D(\theta, \varphi)$ is proportion of any grain on sphere coordinates of film plane, θ and φ are angle of sphere coordinates.

According to the key point 3 of the model, orientation distribution of grain is symmetrical, so the limit of integration of equation (5) is from 0 to 2π, which is corresponding to half integrating sphere. And according to the key point 4 of the model, the orientation distribution of grain is random, so $D(\theta, \varphi)=1$ in equation (5). The Young's modulus of any grain in NPSF is equal to that of single crystalline silicon with same orientation, so [11],

$$Y^i(\theta,\varphi) = [s_{11} - 2(s_{11} - s_{12} - 0.5s_{44}) \times (\sin^4\theta\cos^2\varphi\sin^2\varphi + \sin^2\theta\cos^2\theta)]^{-1} \tag{4}$$

Where，$S_{11}=7.68\times10^{-3}$/GPa、$S_{12}=-2.14\times10^{-3}$/Gpa and $S_{44}=12.6\times10^{-3}$/GPa are yield coefficients [12].

Combining the equation (4) into (3), and using the differential transformation between sphere coordinates and rectangular coordinates, it is obtained that the theoretical value of Young's modulus of NPSF is 160.9GPa.

The Young's modulus of NPSF were measured to be about 155~158GPa in experiments, which is very close to the theoretical value 160.9GPa. The theoretical value is consistent with experimental results, which shows that the theory model presented above is valid and the method to calculate the Young's modulus of nano polycrystalline film is just. Because the effect of grain boundary on elastic constant of film is neglected, theoretical value is slightly larger than experimental results.

5. Conclusion

(1) The Young's modulus of NPSF were measured to be about 155~158GPa in experiments, which is very close to the theoretical value 160.9GPa. The theory model presented in this paper can analyses the Young's modulus of nano polycrystalline film materials.

(2) Further complementing studies about mechanics properties of NPSF will be our next work, which can help us to take good advantage of the NPSF.

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